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Optically detected electron paramagnetic resonance and infrared spectroscopy have been used to probe the microscopic properties of defects in GaN. Irradiation of GaN by 2.5 MeV electrons, *in situ* at 4.2 K, produces two ODEPR signals that have been assigned to interstitial Ga in two distinct configurations. Models for these configurations and interconversion between them are proposed. In separate experiments, the implantation of protons into GaN, *in situ* at 20 K, produces a new H vibrational line at 1456 cm^{-1}. This defect has been associated with isolated H in GaN and provides clues about the structure and mobility of H.

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Defects, GaN, magnetic resonance, IR spectroscopy

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Defects and Defect Processes in GaN

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Abstract: Optically detected electron paramagnetic resonance and infrared spectroscopy have been used to probe the microscopic properties of defects in GaN. Irradiation of GaN by 2.5 MeV electrons, *in situ* at 4.2 K, produces two ODEPR signals that have been assigned to interstitial Ga in two distinct configurations. Models for these configurations and interconversion between them are proposed. In separate experiments, the implantation of protons into GaN, *in situ* at 20 K, produces a new H vibrational line at 1456 cm^{-1}. This defect has been associated with isolated H in GaN and provides clues about the structure and mobility of H.

A. Native defects in GaN

In experiments performed by Watkins and a postdoctoral researcher, two distinct configurations were observed by optical detection of electron paramagnetic resonance (ODEPR) for interstitial Ga^{++} in GaN, as produced by 2.5 MeV electron irradiation *in situ* at 4.2 K. Support from ONR has made possible the completion of a careful study of the conversion process between the two, as induced by optical excitation at 1.8 K, and has led to the proposal of two possible models for their configurations. In the first model, the two configurations result from the interstitial in each of the two available sites (T and O) in the wurtzite GaN lattice. In the second model, the two configurations each arise from T-sites, but at different distances from the Ga vacancy from which they were ejected. In either case, conversion between the two sites constitutes a diffusion step, implying athermal recombination-enhanced migration of the interstitial at these cryogenic temperatures. This could have serious implications as to possible degradation mechanisms for GaN devices.

This work was summarized in an invited plenary lecture at the 22nd Int. Conf. on Defects in Semiconductors in Aarhus, Denmark, July, 2003, and a paper was published in the proceedings of this conference. Two Physical Review B articles have been published which summarize the complete picture of what we have learned about the intrinsic defects on the Ga sublattice of GaN.

B. H in GaN and GaAsN alloys

In experiments performed by Stavola and his students that were partially supported by ONR, the properties of H in GaN and in $GaAs_{1-y}N_y$ alloys have been studied by vibrational spectroscopy.

<u>H in GaN.</u> In GaN, protons were implanted at 20K and the defects that are produced were studied prior to warming the sample. (This work was performed in collaboration with Prof. B.

Bech Nielsen, University of Aarhus.) In these experiments, a vibrational line at 1456 cm^{-1} is produced whose properties are consistent with isolated H. The isolated H migrates at 225K where it then interacts with Ga vacancies that are also produced by the implantation to form a family of vacancy-H complexes. These results are the first observation of isolated H in the group-III nitrides and provide the first data on its mobility. These results were reported at the 23rd Int. Conf. on Defects in Semiconductors in Awaji Island, Japan, in July 2005.

H in dilute III-N-V alloys. $GaAs_{1-y}N_y$ alloys have been of great recent interest because of their possible application in multi-junction solar cells and solid-state lasers in the telecommunications wavelength range. For these alloys, unlike for other semiconductors, hydrogen modifies the band gap energy of the material. It has been proposed by several theoretical groups that H forms a dimer defect in these alloys known at H_2^* that is stabilized by the presence of N. This defect was proposed to be the cause of the unusual behavior of H in these materials. We have completed an IR absorption study of hydrogenated $GaAs_{1-y}N_y$ that determined that the principal defect produced by hydrogenation is inconsistent with the properties of H_2^* predicted by theory. These results showed that the behavior of H in these materials was not yet understood in spite of the fact that several theoretical groups had arrived at similar conclusions. Subsequent theoretical work performed at Lehigh (in collaboration with W.B. Fowler) and also by other groups has identified a new defect structure that is consistent with the vibrational properties of the N- and H-containing defects in the dilute III-N-V alloys. A paper on this work was published in Physical Review B.

Publications

1. G. D. Watkins, K. H. Chow, P. Johannesen, L. S. Vlasenko, C. Bozdog, A. J. Zakrzewski, M. Mizuta, H. Sunakawa, N. Kuroda, A. Usui, Intrinsic defects in GaN: what we are learning from magnetic resonance studies, Physica B **340-342**, 25 (2003).

2. K. H. Chow, L. S. Vlasenko, P. Johannesen, C. Bozdog, and G. D. Watkins, A. Usui, H. Sunakawa, C. Sasaoka, and M. Mizuta, Intrinsic defects in GaN. I. Ga sublattice defects observed by optical detection of electron paramagnetic resonance, Phys. Rev. B **69**, 045207 (2004).

3. P. Johannesen, A. J. Zakrzewski, L. S. Vlasenko, G. D. Watkins, A. Usui, H. Sunakawa, C. Sasaoka, and M. Mizuta, Intrinsic defects in GaN. II. Electronically enhanced migration of interstitial Ga observed by optical detection of electron paramagnetic resonance.

4. F. Jiang, M. Stavola, M. Capizzi, A. Polimeni, A. Amore Bonapasta, and F. Filippone, Vibrational spectroscopy of hydrogenated GaAsN: A structure sensitive test of an H_2^* model, Phys. Rev. B **69**, 041309 (2004).